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DIRECT SAMPLING OF MONTE CARLO FLIGHT PATHS IN MEDIA WITH CONTINUOUSLY VARYING CROSS-SECTIONS

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ABSTRACT

A new Monte Carlo technique has been developed for the direct sampling of flight paths in media with continuously varying cross-sections. This technique provides an alternative to the use of delta-tracking for problems where the material cross-sections vary over the particle flight paths. The technique is general, and may provide benefits to Monte Carlo calculations of charged particles, atmospheric transport, charge transport in semiconductors, radiative transfer for ICF and astrophysics, and transport through stochastic media.

Key Words: Monte Carlo, random sampling

1. INTRODUCTION

There are many classes of Monte Carlo problems where the material cross-sections vary continuously within a geometric region. Examples include: radiation transport through the atmosphere [1], where density varies with position; radiation transport through clouds [2], where the cloud-particle distribution varies with position; time-dependent radiative transfer calculations for astrophysics and inertial confinement fusion (ICF) [3], where certain numerical schemes introduce an effective scattering cross-section which varies with flight time; charged particle transport using continuous slowing down models [4], where energy (hence cross-sections) change continuously with distance; charge transport in semiconductors [5], where the wave vector changes continuously during a free-flight; transport though stochastic media [6], where the cross-sections vary randomly with position.

The principal difficulty in applying Monte Carlo methods to such problems is the random sampling of particle free-flight distance in media where the cross-sections vary during the particle flights, that is, solving the following equation for the flight distance s:

$$\xi = \int_0^s \Sigma(x) \cdot \exp[-\int_{x_0}^{x} \Sigma(x')dx']\, dx , \tag{1}$$

where ξ is a random number and x denotes position along the particle flight path, which may be curved. One common approach to solving this equation is *substepping*, that is, breaking the flight path into short segments within which the cross-section is assumed constant [4]. This can lead to expensive calculations, since many substeps may be required to retain accuracy when the cross-section variation is large. Another common approach is to solve this equation indirectly using a rejection technique called *delta-tracking* [7,8,9]. This technique dates to the 1960s and is also called pseudo-scattering, hole-tracking, Woodcock tracking, or self-scattering. Delta-tracking uses a fictitious cross-section $\Sigma_{\max}$, chosen or estimated to be the largest value expected during the particle flight. A trial flight distance is sampled using $\Sigma_{\max}$, the particle is moved that distance, and then P= $\Sigma(s)/\Sigma_{\max}$ is determined. With probability P, the flight distance is accepted; with probability 1-P, it is rejected, and the entire procedure is repeated. Delta-tracking is a very powerful Monte Carlo technique, but can suffer from inefficiency if $\Sigma_{\max}$ is much larger than the typical cross-section.

As an alternative to substepping and delta-tracking, we have developed a *direct method* for sampling the free-flight distance for the case of varying cross-sections. This method involves random sampling followed by numerical solution via Newton iteration. The technique has been found to be efficient and is guaranteed to converge. We will provide a detailed description of the new technique, examples of its application to several difficult problems, and a comparison to both the delta-tracking and substepping approaches.

2. THEORETICAL BACKGROUND

Let $\tau(x)$ be the optical depth traversed by a particle traveling a distance x through a medium with arbitrarily specified macroscopic cross-section $\Sigma(x)$:

$$\tau(x) = \int_0^x \Sigma(x')dx' \tag{2}$$

We assume only that $\Sigma(x)$ is finite and $\Sigma(x) \geq 0$. Note that

$$\frac{d\tau}{dx} = \Sigma(x) \tag{3}$$

and $0 \leq d\tau/dx < \infty$. To explicitly allow for the case of no collision in a finite distance of travel, we define P_{NC}, the probability of no collisions, as

$$P_{NC} = e^{-\tau(\infty)} \tag{4}$$

Then the probability density function (pdf) for a collision occuring after a particle has traveled a distance x through the medium is given by

$$f(x) = P_{NC} \cdot \delta(x = \infty) + (1 - P_{NC}) \cdot \frac{1}{G} \cdot \frac{d\tau}{dx} \cdot e^{-\tau(x)} , \tag{5}$$

where G is a normalization constant given by

$$G = \int_0^\infty \frac{d\tau}{dx} \cdot e^{-\tau(x)} dx = 1 - e^{-\tau(\infty)} = 1 - P_{NC}\,, \tag{6}$$

$d\tau/dx$ is the interaction probability per unit distance traveled, $e^{-\tau(x)}$ is probability of traversing distance x without collision, and $0 \le x \le \infty$. Eq. (5) explicitly allows for cases where $\tau(\infty)$ is finite, hence there is a possibility of traveling an infinite distance without colliding. Such cases occur when $\Sigma(x) \to 0$ as $x \to \infty$. (A previous proof of the validity of delta-tracking in [10] assumed that $\tau(\infty) = \infty$, an assumption which was not necessary.) Random sampling of the Monte Carlo flight path requires solving the following equation for s, the flight path:

$$\xi = \int_0^s f(x)dx\,, \quad \text{or} \quad \xi = F(s) \tag{7}$$

where ξ is a uniform random variate in [0,1), *f(x)* is specified by Eqs. (2-6), and *F(x)* is given by

$$F(x) = \int_0^x f(x')dx' = P_{NC} \cdot H(x,\infty) + (1 - P_{NC}) \cdot \frac{1 - e^{-\tau(x)}}{1 - e^{-\tau(\infty)}}\,, \tag{8}$$

with $H(x,\infty)$ the Heaviside step function. Eq. (7) is frequently written as

$$s = F^{-1}(\xi)\,. \tag{9}$$

For the common case required by most Monte Carlo codes, the cross-section is a constant independent of x and Eqs. (2-6) simplify to:

$$\tau(x) = \Sigma x, \quad \frac{d\tau}{dx} = \Sigma, \quad P_{NC} = 0, \quad G = 1, \quad f(x) = \Sigma e^{-\Sigma x} \tag{10}$$

so that Eq. (7) may be readily solved as

$$s = -\ln(1-\xi)/\Sigma \tag{11}$$

Eq. (11) is commonly implemented as $s = -\ln(\xi)/\Sigma$, since ξ and $(1-\xi)$ have equivalent uniform distributions. For media where $\Sigma(x)$ varies, Eq. (7) may be difficult or impossible to solve analytically.

3. DIRECT SAMPLING TECHNIQUE FOR FREE-FLIGHT DISTANCE

Examination of Eq. (5) shows that Eq. (7) is readily solved via a 2-stage sampling procedure: First, discrete sampling is used to select a collision with probability $(1\text{-}P_{NC})$ or an infinite flight with probability P_{NC}. That is,

If $\xi \le P_{NC}$,

No collision: select $s = \infty$

Otherwise,

Collision: sample s from $g(x) = \frac{1}{G} \cdot \frac{d\tau}{dx} \cdot e^{-\tau(x)}$

For the case where a collision does occur, then the second step involves sampling s from the pdf given by:

$$g(x) = \frac{1}{G} \cdot \frac{d\tau}{dx} \cdot e^{-\tau(x)}\,, \tag{12}$$

where $0 \le x < \infty$. Using Eq. (12), we note that

$$\int_0^s g(x)dx = \frac{1}{G} \cdot \int_0^{\hat{\tau}} e^{-\tau} d\tau , \tag{13}$$

with $\hat{\tau}$ defined by $\hat{\tau} = \tau(s)$. Then, using Eqs. (7) and (13), we can sample $\hat{\tau}$ by solving

$$\xi = \frac{1}{G} \int_0^{\hat{\tau}} e^{-\tau} d\tau \tag{14}$$

with $0 \le \hat{\tau} < \tau(\infty)$. This is equivalent to sampling $\hat{\tau}$ from a truncated exponential pdf, which has the solution

$$\hat{\tau} = -\ln(1 - G \cdot \xi) \tag{15}$$

Substituting $\hat{\tau}$ for τ, and s for x in Eq. (2) gives:

$$\hat{\tau} = \int_0^s \Sigma(x) dx \tag{16}$$

When $\Sigma(x)$ has a simple functional form, Eq. (16) can often be solved analytically for s. In many cases which arise in practice, the solution may involve a transcendental equation or other form not amenable to analytic solution. Eq. (16), however, can be readily solved numerically for s using Newton iteration:

$$\begin{aligned}
& s_0 = \hat{\tau} / \Sigma(x_0) \\
& n = 0 \\
& \text{Iterate:} \\
& \qquad n = n + 1 \\
& \qquad g = \hat{\tau} - \tau(s_{n-1}) \\
& \qquad g' = dg/ds = -\Sigma(x_0 + s_{n-1}) \\
& \qquad s_n = s_{n-1} - g / g' \\
& \qquad \text{Stop if } |s_n - s_{n-1}| < \varepsilon
\end{aligned} \tag{17}$$

Because $g' \le 0$ in Eq. (17), $g(s)$ is monotone and there can be at most one root of Eq. (16). For cases where $\Sigma(x)$ is always greater than 0, the Newton iteration in Eq. (17) is guaranteed to converge. However, if $\Sigma(x)$ is zero or very small over a portion of the flight path, g' may be 0 in Eq. (17), leading to numerical difficulties and nonconvergence. This potential problem is remedied easily by combining Eq. (17) with a bisection search method, such that Eq. (17) is used when g' is nonzero and bisection is used if g' is very small or zero. Using this approach, we have found that only 1-5 iterations in Eq. (17) are typically needed to converge s to within 10^{-6}, even for extreme variations in $\Sigma(x)$.

4. NUMERICAL RESULTS

4.1 Verification of Direct Numerical Sampling

To verify that the analysis and proposed sampling method in Section 3 are correct, we have applied the method to the Monte Carlo transport of particles through a 1-D slab of thickness 2 units. We consider only transmission through the slab, ignoring scattering. Table I shows 7 different forms of spatial variation in the cross-section which were used for the test problem. Figures 1 through 7 show the cross-section variation over the thickness of the slab (labeled "sig"), the pdf at position *x=0* given by Eq. (12) for the cross-section variation in each test case (labeled "pdf"), and the results of using the direct numerical sampling procedure from Section 3 to perform 1,000,000 samples of the free-flight distance for each case (labeled "sampled"). The sampled results were binned in 100 bins of width 0.02. In Figures 1-7, it can be seen that the distributions of sampled results for the free-flight distance agree completely with the exact pdf's in all cases, verifying that the sampling method in Section 3 is correct.

Table I. Cross-section Variation for Test Cases

Case	Cross-section Variation	Numerical Representation, for range $0 \le x \le 2$
1	Constant	$\Sigma(x) = 1$
2	Linearly Decreasing	$\Sigma(x) = 2 - x$
3	Linearly Increasing	$\Sigma(x) = x$
4	Exponentially Decreasing	$\Sigma(x) = \exp(-3x)$
5	Exponentially Increasing	$\Sigma(x) = 0.1 \cdot \exp(2x)$
6	Sharp Gaussian	$\Sigma(x) = \frac{2}{\sqrt{2\pi}} \exp\left[-\left(\frac{x-1}{0.05} \right)^2 \right]$
7	Broad Gaussian	$\Sigma(x) = \frac{2}{\sqrt{2\pi}} \exp\left[-\left(\frac{x-1}{1.0} \right)^2 \right]$

4.2 Comparison of Direct Numerical, Delta-tracking, and Substepping Methods

We have also compared the effectiveness of the direct numerical sampling procedure to the delta-tracking and substepping methods for the same 7 cases of cross-section variation given in Table I. In these tests, multiple collisions were followed and the resulting transmission through the slab was computed for each test case, using direct numerical sampling, delta-tracking, and substepping. For delta-tracking, the actual value of the maximum cross-section over the interval was used, rather than an arbitrary guess. For the substepping method, equal-thickness subdivisions of the slab were used, with the number of subdivisions determined by trial and error to be the minimum required to match the accuracy of the other two methods. That is, if the transmission through the slab did not match that from delta-tracking or the direct method (within statistics), the number of subdivisions of the slab was increased by 5 and the calculations repeated. 1,000,000 histories were followed for each method in each of the test cases. The results of these comparisons are given in Table II.

In Table II it can be seen that the accuracy of all 3 methods is comparable, given that sufficient substeps are used for the substepping method. The number of collisions and the transmission at the right slab boundary are the same within statistics for all 3 methods. (The statistics are not shown in the table, but the standard deviations for number of collisions are simply the square root of the results, and the standard deviations of the transmission are the square root of the results divided by 1,000, since all calculations were run in strict analog fashion.)

Table II. Comparison of Direct Numerical, Delta-Tracking, and Substepping Methods

Method	Collisions	Transmission	Function Evaluations per Collision
1. Constant Cross-section			
Substep	865001	0.1350	2.16
Delta-tracking	865362	0.1354	1.00
Direct	864513	0.1355	1.00
2. Linearly Decreasing			
Substep	865189	0.1348	29.90
Delta-tracking	865362	0.1346	1.48
Direct	865145	0.1349	2.95
3. Linearly Increasing			
Substep	864742	0.1353	29.92
Delta-tracking	864754	0.1352	2.77
Direct	864998	0.1350	4.38
4. Exponentially Decreasing			
Substep	282293	0.7177	107.08
Delta-tracking	283236	0.7168	5.37
Direct	282881	0.7171	3.78
5. Exponentially Increasing			
Substep	931436	0.0686	33.20
Delta-tracking	931279	0.0687	7.55
Direct	931884	0.0681	4.94
6. Sharp Gaussian			
Substep	864591	0.1354	41.17
Delta-tracking	864494	0.1355	20.53
Direct	864518	0.1355	4.06
7. Broad Gaussian			
Substep	745446	0.2546	27.84
Delta-tracking	745301	0.2547	1.18
Direct	744956	0.2550	3.26

The column in Table II labeled “Function Evaluations per Collision” represents the average number of flights per collision for the substepping method, the average number of pseudo-collisions (delta + real) for each real collision for the delta-tracking method, and the average number of Newton iterations per collision for the direct numerical method. These are useful numbers to compare in assessing the effectiveness of each method: Each of these actions (substep, pseudo-collision, Newton iteration) involves one evaluation of the cross-section function and a few arithmetic or logical operations. It is not feasible to simply measure the CPU time required for these actions, since CPU time is highly variable depending on the problem geometry, complexity of the cross-section variation and evaluation routines, etc. It is more meaningful to assess the three methods algorithmically for the 7 test cases. The last column in Table II provides a good measure of the effectiveness of the three methods for sampling the free-flight distance, irrespective of other details of the Monte Carlo code.

In examining Table II it can be seen that both delta-tracking and the direct method are significantly more effective than substepping if the cross-sections vary within a region. Substepping typically requires 20 or more substeps (for these test cases), making it far more costly than the other two methods. Delta-tracking and the direct method are roughly comparable, with delta-tracking being faster when there is little variation in the cross-section and the direct method being faster when there is more variation in the cross-section. In general, the direct method should be viewed as an alternative to delta-tracking if there are large variations in cross-section. However, it should be noted that the direct method is competitive with delta-tracking even for those cases where the cross-section does not vary much. In Case 7, for example, delta-tracking is 3 times more effective than the direct method, while in Case 6 the direct method is about 5 times more effective. For cases where the maximum cross-section is not known and must be estimated, such as in electron transport with energy-varying cross sections, the direct method may offer substantial advantages compared to delta tracking or substepping.

5. CONCLUSIONS

Traditional Monte Carlo approaches to problems where the cross-section varies spatially or temporally along the particle flight path have involved either substepping or delta-tracking. We have provided an alternate method for such problems, direct numerical solution, which can be more effective than either method for certain classes of cross-section variation. Numerical testing has verified the correctness of the method. Numerical comparisons between the direct, substepping, and delta-tracking methods have been made for 7 different functional forms of cross-section variation. Both the direct and delta-tracking methods were shown to be more effective than substepping in all cases. For sharply peaked or strongly varying cross-sections, the direct method is preferable to delta-tracking.

Finally, it should be noted that the type of tallies desired for the Monte Carlo calculation may be a decisive factor in any decision between delta-tracking and the direct method. Delta-tracking does not involve the calculation of distances nor the integral of the cross-section along the flight path, which is required information if pathlength tallies are desired. Indeed, delta-tracking is often used precisely in those problems where such path-integral information is hard to obtain. This information, however, is inherent in the direct method and is determined numerically, so that difficult functional forms for the variation in cross-section are handled as easily as simple ones. Thus pathlength tallies are essentially free when the direct method is used. Since pathlength tallies frequently have lower variance than collision or pseudo-collision tallies, the effective cost in terms of the figure-of-merit (i.e., FOM=1/(variance x CPU time)) [4] of using the direct method may in practice be lower than the comparisons in this paper would indicate. Future work on the direct numerical method should examine this issue.

REFERENCES

1. CJ Everett, ED Cashwell, RG Schrandt, "A Monte Carlo Transport Routine for the 'US Standard Atmosphere' (1962) to an Altitude of 90 Kilometers," LA-5089-MS, Los Alamos National Laboratory (1972).
2. G.E. Thomas and K. Stamnes, Radiative Transfer in the Atmosphere and Oceans, p. 429, Cambridge University Press (1999).
3. W.R. Martin and F.B. Brown, "Comparison of Monte Carlo Methods for Nonlinear Radiation Transport," *Proc. ANS Mathematics and Computations Topical Meeting*, Salt Lake City (Sept 2001).
4. J.F. Briesmeister, Ed., "MCNP – A General Monte Carlo N-Particle Transport Code – Version 4C," LA-13709-M, Los Alamos National Laboratory (2000).
5. H.D. Rees, *Phys. Lett. A* **26**, 416 (1968), also *J. Phys. Chem. Solids* **30**, 643 (1969).
6. M.M.R. Williams, Random Processes in Nuclear Reactors, Pergamon Press (1974).
7. E.R. Woodcock, T. Murphy, P.J. Hemmings, T.C. Longworth, "Techniques Used in the GEM Code for Monte Carlo Neutronics Calculations in Reactors and Other Systems of Complex Geometry," *Proc. Conf. Applications of Computing Methods to Reactor Problems*, ANL-7050, p. 557, Argonne National Laboratory (1965).
8. L. L. Carter, E. D. Cashwell, & W. M. Taylor, "Monte Carlo Sampling with Continuously Varying Cross Sections Along Flight Paths", *Nucl. Sci. Eng.* **48**, 403-411 (1972).
9. S.N. Cramer, "Application of the Fictitious Scattering Radiation Transport Model for Deep-Penetration Monte Carlo Calculations," ORNL/TM-4880, Oak Ridge National Laboratory (1977).
10. W.A. Coleman, "Mathematical Verification of a Certain Monte Carlo Sampling Technique and Applications of the Technique to Radiation Transport Problems," *Nucl. Sci. Eng.* **32**, 76-81 (1968).

Figure 1. Constant Cross-section

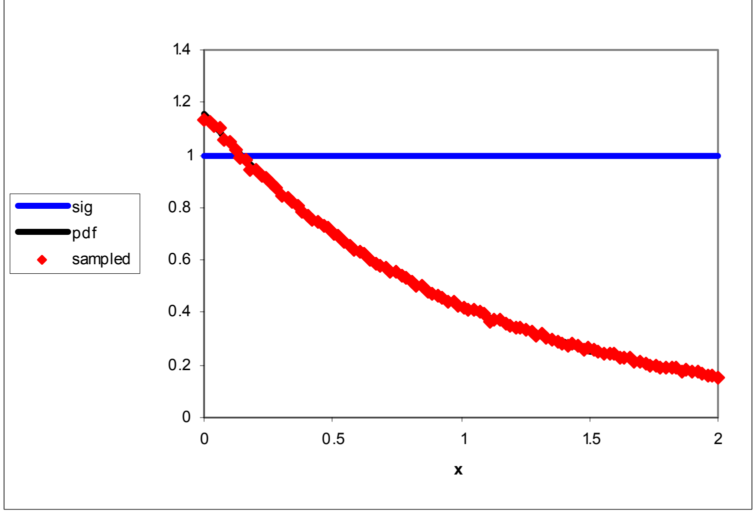


Figure 2. Linear Decrease

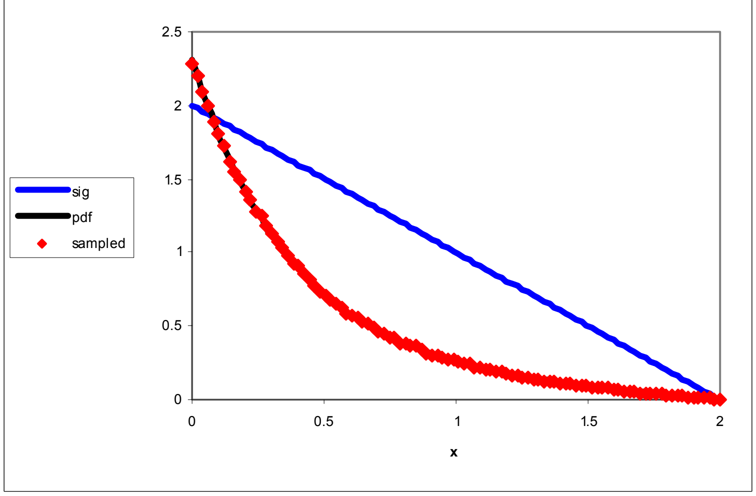
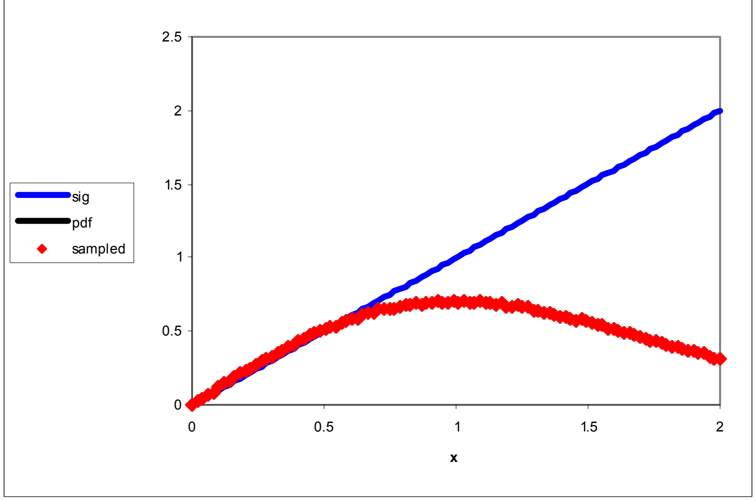


Figure 3. Linear Increase



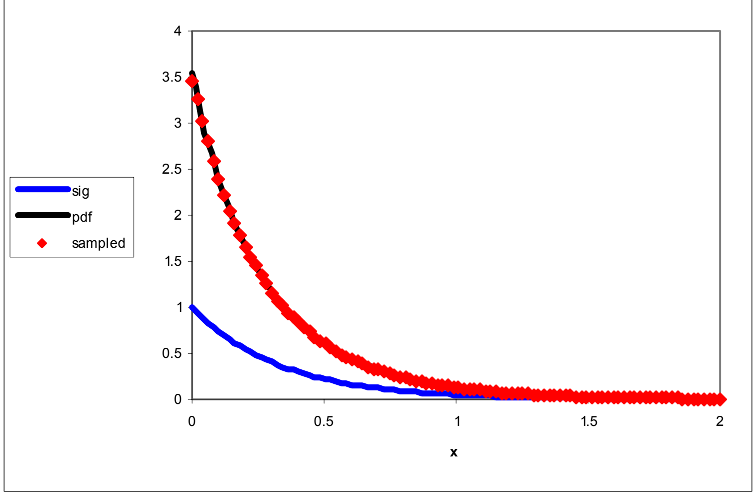


Figure 4. Exponential Decrease

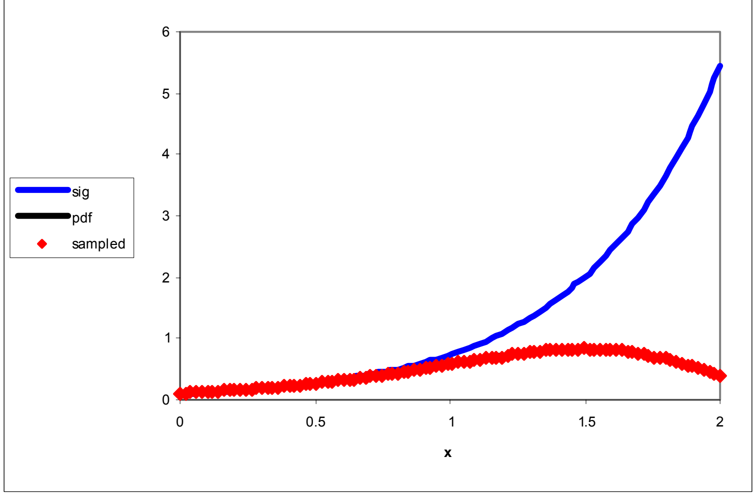


Figure 5. Exponential Increase

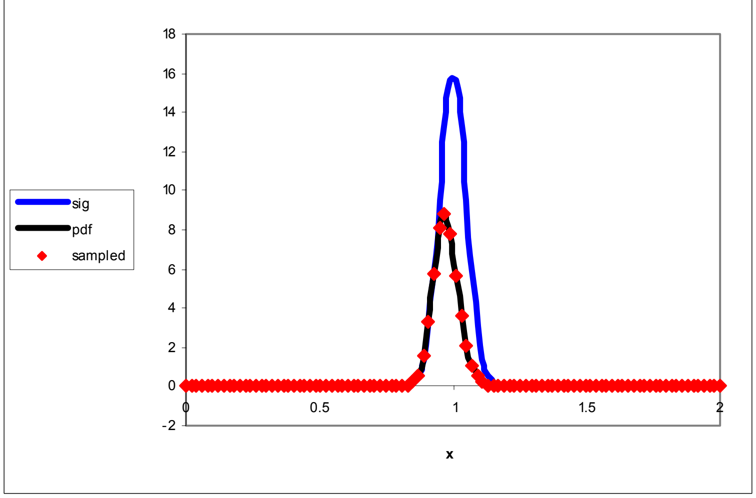


Figure 6. Sharp Gaussian

Figure 7. Broad Gaussian